Supplementary material for the article:

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Tautomerism of 4-phenyl-2,4-dioxobutanoic acid. Insights from pH ramping NMR study and quantum chemical calculations

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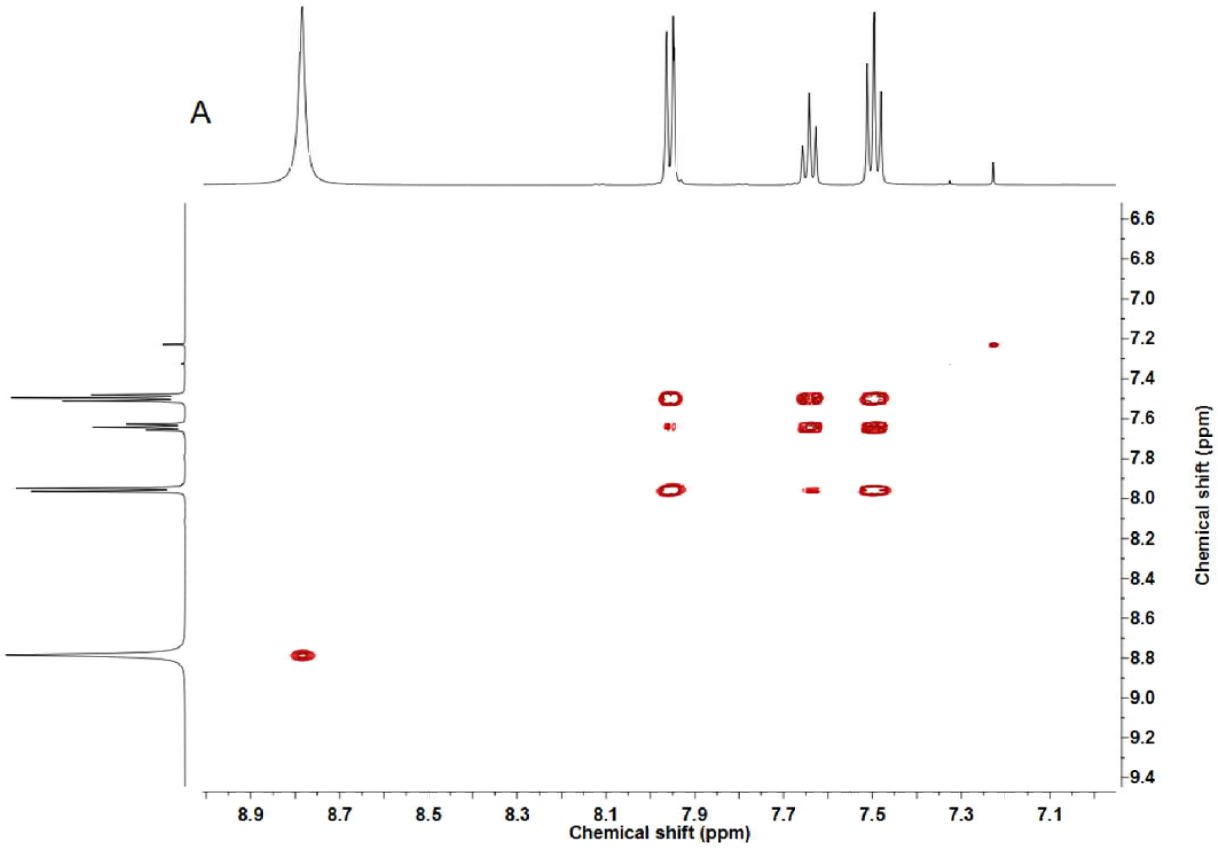

Fig. S1 A) COSY spectrum of 4PDA in CD_3COOD (pH<0); t=25±1 °C; I=0.1 M ($NaNO_3$)

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& We regret to inform that Branko Drakulić has passed away since completion of this work.

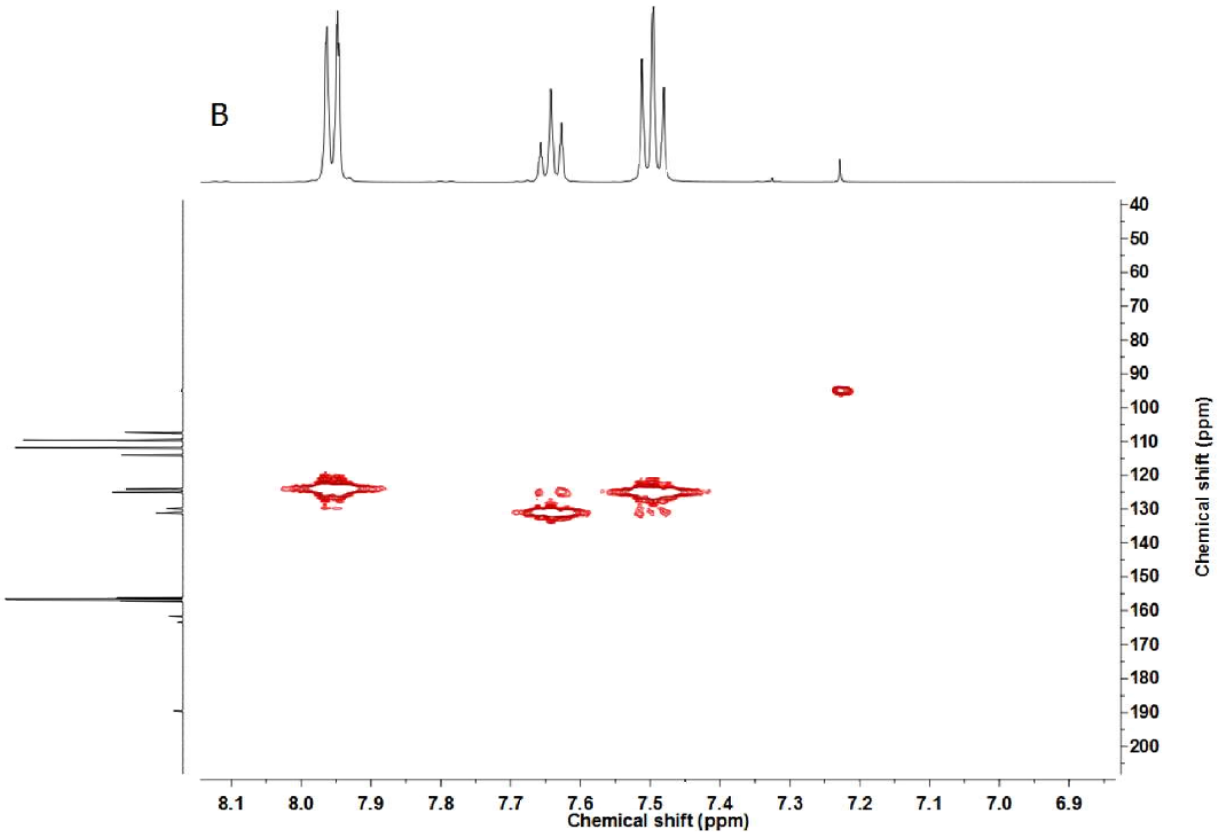

Fig. S1 B) HMQC spectrum of 4PDA in CD_3COOD (pH<0); t=25±1 °C; I=0.1 M ($NaNO_3$).

Table S1. Dipole moments of all tautomers of 4PDA, calculated with MP2/6-31G(d,p) Hamiltonian in vaccum, implicit solvation model (water), and with explicitly bound single water molecule

Tautomer	**μ** $_{vacuum}$ **(Debye)**	**μ** $_{impl.\ solvent}$ **(Debye)**	**μ** $_{one\_water}$ **(Debye)**
diketo **II** *out*	3.8253	5.5027	5.6150
diketo **II** *in*	5.3744	6.7330	5.6905
enol **I** *out*	2.7033	3.4447	4.1323
enol **I** *in*	4.4432	4.9796	4.7665
enol **III** *out*	2.9839	3.7212	4.3209
enol **III** *in*	5.2227	6.0376	8.2546